

1500
IR

C₄H₂

1,3-Butadiyne
Diacetylene

D_{∞h}
H-C≡C-C≡C-H

r_0	Å
C-H	1.058(5) ^{a)}
C≡C	1.205(5) ^{a)}
C-C	1.378(5) ^{a)}

Bond lengths transferred from HC₃N predict a B_0 value extremely close (0.08%) to the experimental one. Therefore, the geometric parameters should be very close to the transferred distances. This is further confirmed by *ab initio* predictions.

^{a)} Distances are taken from HC₃N. Uncertainties were not estimated in the original paper.

McNaughton, D., Bruget, D.N.: J. Mol. Struct. **272** (1992) 11.

ED

r_g	Å ^{a)}
C-H	1.0935(100)
C≡C	1.2176(14)
C-C	1.3837(19)

The rotational constant B_0 estimated from the r_g distances is smaller than the spectroscopic value by about 0.8%. This difference is probably due to a bending-stretching interaction; i.e., bonds are slightly stretched when they are bent [1].

The measurements were made at room temperature.

^{a)} Estimated limits of error.

Tanimoto, M., Kuchitsu, K., Morino, Y.: Bull. Chem. Soc. Jpn. **44** (1971) 386.

[1] Ohshima, Y., Yamamoto, S., Kuchitsu, K.: Acta Chem. Scand. Ser. A **42** (1988) 307.